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Burnup calculations using serpent code in accelerator driven thorium reactors

In this study, burnup calculations have been performed for a sodium cooled Accelerator Driven Thorium Reactor (ADTR) using the Serpent 1.1.16 Monte Carlo code. The ADTR has been designed for burning minor actinides, mixed ^{232}Th and mixed ^{233}U fuels. A solid Pb-Bi spallation target in the center of the core is used and sodium as coolant. The system is designed for a heating power of 2000 MW and for an operation time of 600 days. For burnup calculations the Advanced Matrix Exponential Method CRAM (Chebyshev Rational Approximation Method) and different nuclear data libraries (ENDF7, JEF2.2, JEFF3.1.1) were used. The effective multiplication factor can increase from 0.93 to 0.97 for different nuclear data libraries during the reactor operation period.

Abbrandrechnungen mit Hilfe des Serpent Codes für beschleunigergetriebene Thorium-Reaktoren. *In dieser Arbeit wurden Abbrandrechnungen für einen Natrium-gekühlten beschleunigergetriebenen Thorium-Reaktor (ADTR) mit Hilfe des Monte-Carlo Codes Serpent 1.1.16 durchgeführt. Der ADTR wurde ausgelegt für minore Aktinide, gemischte ^{232}Th und ^{233}U Brennstoffe. Im Zentrum des Kerns wurde ein Pb-Bi Target und als Kühlmittel Natrium verwendet. Das System wurde ausgelegt für eine Heizleistung von 2000 MW und eine Betriebszeit von 600 Tagen. Für die Abbrandberechnungen wurden die Advanced Matrix Exponential Method CRAM (Chebyshev Rational Approximation Method) und verschiedene Kerndatenbibliotheken (ENDF7, JEF2.2, JEFF3.1.1) verwendet. Der effektive Multiplikationsfaktor kann sich während der Betriebszeit von 0.93 auf 0.97 erhöhen je nach Kerndatenbibliothek.*

1 Introduction

The present knowledge of thorium resources has been limited in the world and research continues on the subject. Apart from its main use in nuclear energy as "fertile" material, the use of thorium as nuclear fuel is limited. Thorium and uranium are the two heaviest elements occurring in nature for nuclear fission energy. Thorium is three times more abundant compared to uranium in nature. Thorium fuels have not been commercially developed because the estimated uranium resources turned out to be sufficient. The thorium fuel cycle has several unique issues, both for "open" and "closed" cycles, which need to be addressed and resolved before thorium could be introduced in Accelerator Driven Systems. The closed $^{232}Th/^{233}U$ fuel cycle should be developed on an industrial scale for most efficient use of thorium resources. Accelerator Driven Reactors convert material like ^{232}Th and ^{238}U into fissionable material like ^{233}U and ^{239}Pu [1]. The $^{232}Th/^{233}U$ fuel cycle has the added advantage that it minimizes the production of long-lived actinide waste. The reactors, which produce more fissionable material than they consume are called breeder reactors [2].

There is a lack of experience and know-how on the back end issues of high burnup in once-through $^{232}Th/^{233}U$ and Th minor actinides fuel cycles and multiple recycling of Th, U and Pu. In addition, there are the common challenges for thorium and uranium fuel cycles like annihilation of long lived radionuclides by transmutation into stable or short lived products. Thorium fuels are an attractive way to produce long term nuclear energy. In addition, the thorium fuel cycles could be done through the incineration of radiotoxicity waste. However, there are several challenges related to thorium fuel cycles. The $^{232}Th-^{233}U$ fuel cycle can operate with fast, epithermal or thermal spectra and ^{233}U can be used for breeding in both thermal and fast reactors [3, 4].

In recent decades, thorium fuels have been investigated because of attractive features of Accelerator Driven Thorium Reactors (ADTR). ADTR offer potentially significant advantages in once-through or closed fuel cycle for the fuel breeding. Protons with high energy are collided with Pb or Pb–Bi alloy targets to produce spallation neutrons [5, 6].

Plutonium (Pu) and the minor actinides (MA), such as Neptunium (Np), Americium (Am) and Curium (Cm), accumulated in the spent nuclear fuel of LWR are very hazardous components of long-life nuclear waste. Thorium based fuel cycles do not produce minor actinides and the use of thorium fuels with minor actinides in ADTR have a potential to reduce nuclear waste [7].

2 ADTR system

In order to operate thermal nuclear reactors moderate neutrons to low energy and consume fissile isotopes. But neutrons are not slowed down in fast reactors which produce more fissionable material than they consume are called Accelerator Driven Thorium Reactors (ADTR).

The main objective of Accelerator Driven Systems (ADS) is providing long term solutions to nuclear waste disposal by burning plutonium, minor actinides and transmutation of long lived fission products. The main advantage of ADS is to become subcritical over conventional nuclear systems, which allows for larger reactivity margin independent of the delayed neutron fraction. The accelerator may provide a convenient control mechanism for subcritical systems that would eliminate the need of control rods. The ADTR consists of three components (i) the proton accelerator, (ii) the target (Pb or Pb–Bi alloy), and (iii) a sub-critical reactor core of neutron multiplication factor in the range of 0.95–0.98. The aim of ADTR is to bombard a subcritical fuel mixture (U, Th, Pu …) with fast neutrons coming from a spallation source induced by an accelerator (Linac or Cyclotron). In addition, the ADTR has heat removal and electricity generation equipment [8].

In various ADS applications, the solid Lead-Bismuth or a eutectic of Lead-Bismuth has been the focus of attention both as spallation targets. The ADS is controlled through reactions in the spallation target which is caused by the proton current [9, 10]. The deficiency of neutrons is compensated by the spallation neutron source in the subcritical core of the ADS [11]. Spallation reactions are generally described by a two stage. The intranuclear cascade model is generally described by the first step while second step is described by evaporation fission model [12, 13].

3 Serpent code

Monte Carlo method is a statistical method. It is particularly useful for complex problems that cannot be solved by deterministic methods. The examination of reactor criticality was among the important problems to which Monte Carlo methods were applied. The fundamental question is the behavior of large numbers of neutrons inside the reactor. In fact, when neutrons travelling in the moderator are scattered, or when a neutron is absorbed in a uranium atom with a resultant fission event, particles fly off in random directions according to the appropriate differential cross sections. Monte Carlo codes are well suited for criticality safety analyses, radiation shielding and dosimetry calculations, detector modeling in complicated three-dimensional geometries [14].

Serpent is a new continuous-energy Monte Carlo reactor physics code, developed at VTT under the working title "Probabilistic Scattering Game". The Serpent code is mainly intended for lattice physics calculations [15]. Serpent uses ENDF format interaction data, read from ACE format cross section libraries. Burnup calculations require radioactive decay data and neutron-induced and spontaneous fission product yields. These files are read in the raw ENDF format [16].

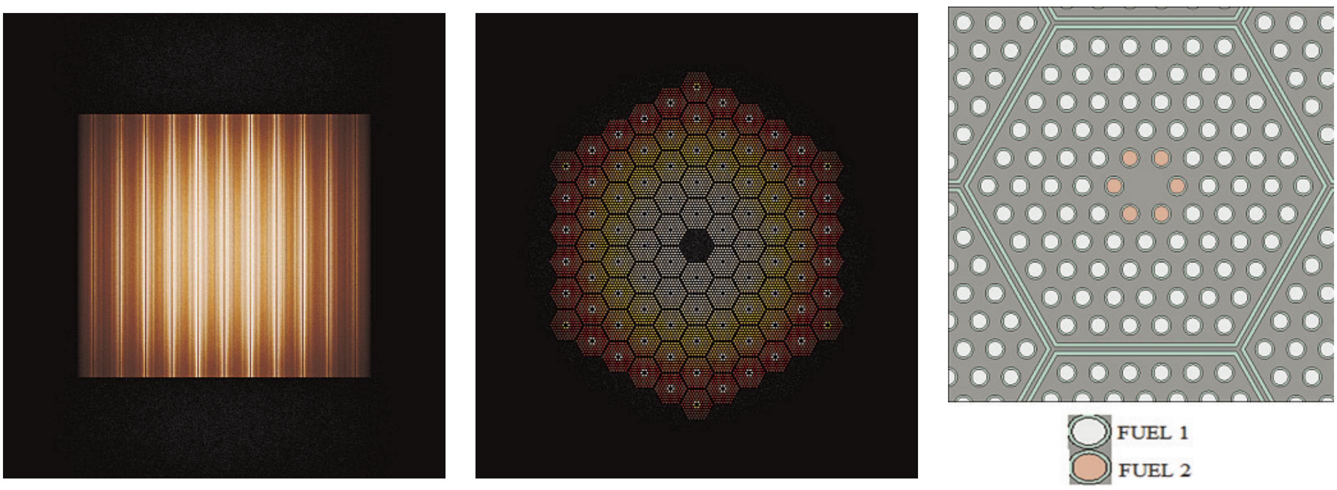
Three types of cross sections are available in the data files. First, continuous-energy neutron cross sections contain all necessary reaction cross sections, together with energy and angular distributions, fission neutron yields and delayed neutron parameters for the actual transport simulation. Second, dosimetry cross sections exist for a large variety of materials and can be used with detectors but not in physical materials included in the transport calculations. Third, thermal scattering cross sections are used to replace the low-energy free-gas elastic scattering reactions for some important bound moderator nuclides. All calculation outputs are written in Matlab files (m-format) to simplify the simultaneous post-processing of several calculation cases. The code also has a geometry plotter feature and a reaction rate mesh plotter [17].

4 Advanced matrix exponential method: CRAM

Serpent code uses an internal calculation routine for solving the set of Bateman equations describing the changes in the material compositions caused by neutron induced reactions and radioactive decay and the code is used as the neutronics solver in an externally coupled system. Serpent code has three methods for solving the Bateman equations describing the changes in the isotopic compositions caused by neutron-in-

Table 1. The main materials in the ADTR structure

	Isotopes in the material
Fuel 1	^{232}Th; ^{237,238,239}U; ^{235,236,237,238,239}Np; ^{239,240,241,242,243,244}Pu; ^{241,242,243}Cm; ^{135}Xe; ^{62}Sm; ^{106}Pd; ^{92}Zr
Fuel 2	^{233}U; ^{237,238,239}U; ^{235,236,237,238,239}Np; ^{239,240,241,242,243,244}Pu; ^{241,242,243}Cm; ^{135}Xe; ^{62}Sm; ^{106}Pd; ^{92}Zr
Cooled	^{23}Na
Target	^{206,207,208}Pb; ^{209}Bi
Clad (Steel)	^{12}C; ^{27}Al; ^{28,29,30}Si; ^{31}P; ^{32}S; ^{51}V; ^{50,52,53,54}Cr; ^{55}Mn; ^{54,56,57,58}Fe; ^{63,65}Cu; ^{96}Mo; ^{182,183,184,186}W



(a) (b) (c)

Fig. 1. (a) Vertical mesh results, (b) Horizontal mesh results of ADTR design and (c) the horizontal view of the a for Fuel 1 and Fuel 2

duced reactions and radioactive decay. The first method is the Transmutation Trajectory Analysis (TTA), based on the analytical solution of linearized transmutation chains [18]. The second method, used by default, is an advanced matrix exponential solution based on the Chebyshev Rational Approximation Method (CRAM). The third option is the variation TTA method, in which cyclic transmutation chains are handled by inducing small variations in the coefficients instead of solving the extended TTA equations [19].

The changes in material compositions and neutronic properties in a reactor fuel are taken into account in all reactor physics calculations by burnup calculation codes. Various methods exist for performing these calculations. An advanced matrix exponential solution based on the Chebyshev Rational Approximation Method (CRAM) is used in solution of depletion equations by default. The one of advantage is capable of providing accurate solution to the burnup equations with a very short computation time [20].

CRAM is capable of providing a robust and accurate solution to the burnup equations. This method is based on the solution of burnup matrix containing the decay and transmutation coefficients of the nuclides in the irradiated material [21].

Table 2. The geometry specifications of the ADTR system

Pin numbers in each assembly	90
Total assembly numbers in system	90
Total pin number in system	8100
Fuel pin height and radius	200 cm – 0.75 cm
Target height and radius	60 cm – 15 cm
System height and radius	460 cm – 230 cm

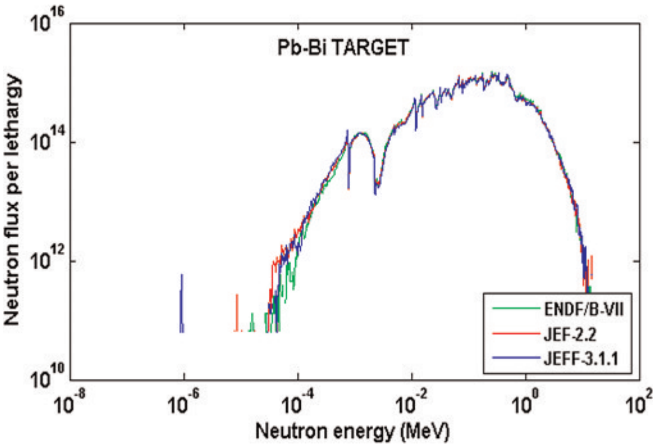


Fig. 2. Neutron flux per lethargy in the Pb–Bi target

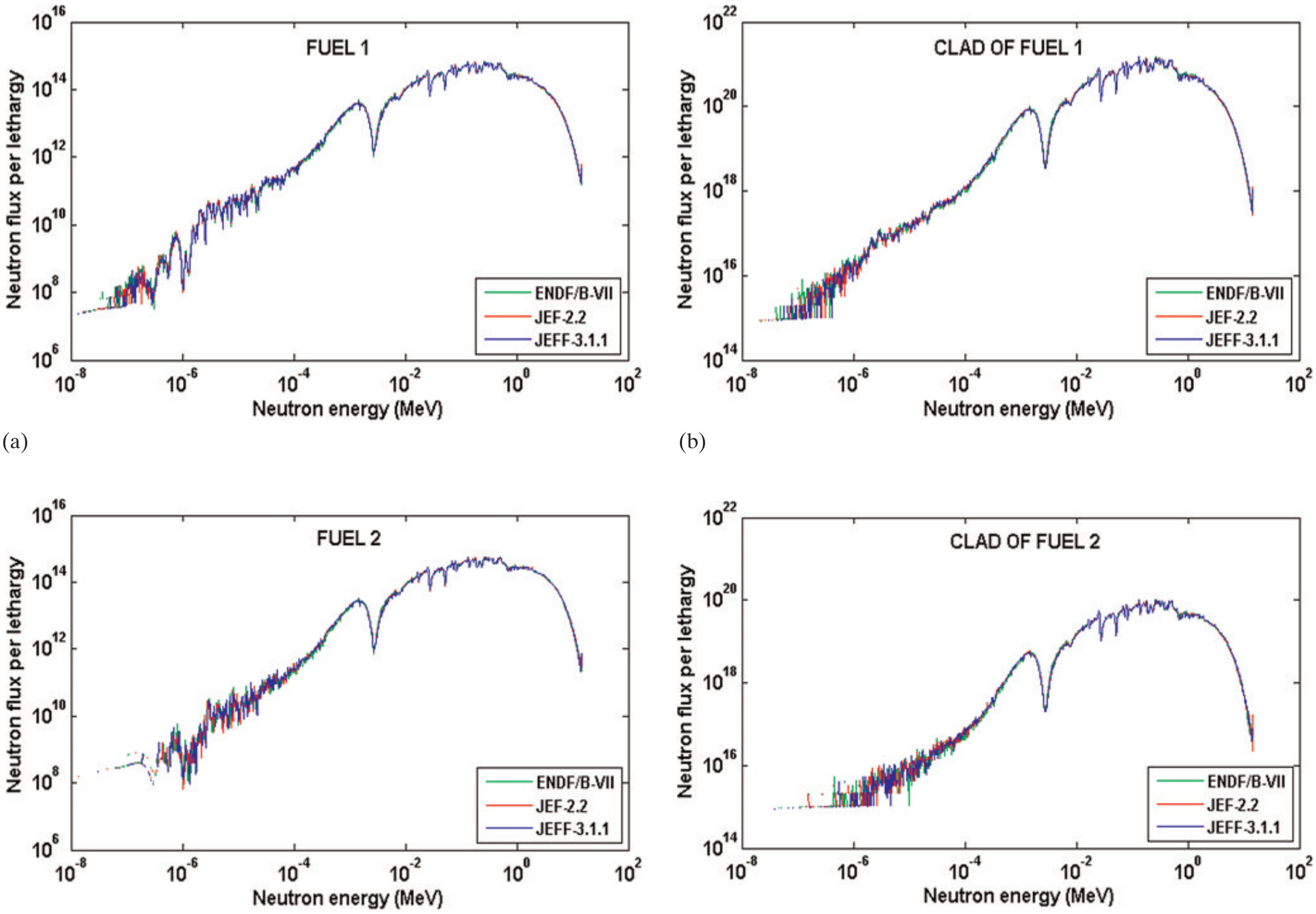


Fig. 3. Neutron flux per lethargy for (a) fuel 1, (b) clad of fuel 1 and (c) fuel 2, (d) clad of fuel 2

5 Reactor design description

All the calculations in this work were performed using the Serpent 1.1.16 Monte Carlo code. A number of simulations were performed using Serpent in order to obtain neutronic and burn-up characteristics of the ADTR models. ADTR have been designed in these calculations by using Serpent geometry plotter. Table 1 describes the construction materials and fuels. Fuel 1 rods (Fuel 1) are composed of ^{232}Th and minor actinides. There are ^{233}U and other fuel isotopes in Fuel 2. The target material is lead-bismuth. As coolant and moderator liquid sodium was chosen for its excellent thermal properties. The construction materials of the fuel rods were made of steel. Table 1 below describes the ADTR material structure. The distributions of the pin cell are shown in Fig. 1 as white pin (Fuel 1) and pink pin (Fuel 2). The two dimensional geometry of the system and mesh plot is shown in Fig. 1. There are 540 fuel 1 rods, 7560 fuel 2 rods in the system. Figure 1 shows the reaction rate mesh plotter results in 2D model. The mesh calculations were used in thermal analysis for visualizing the coupling between neutron flux and fission rate in the Serpent code. The geometry specifications of the ADTR system are shown in Table 2.

6 Neutronic and burnup calculations

The neutronic behaviors of ADTR have been investigated in target and fuel pins using different data libraries. As cross sec-

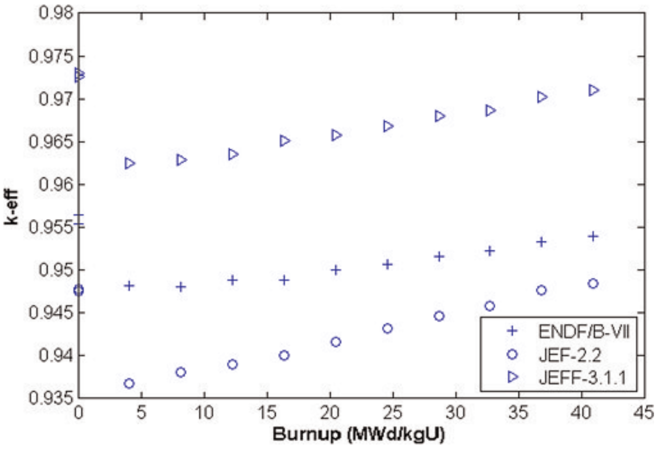
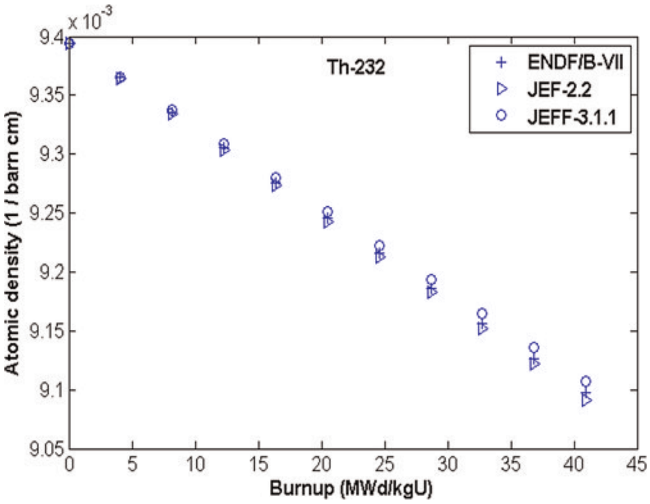
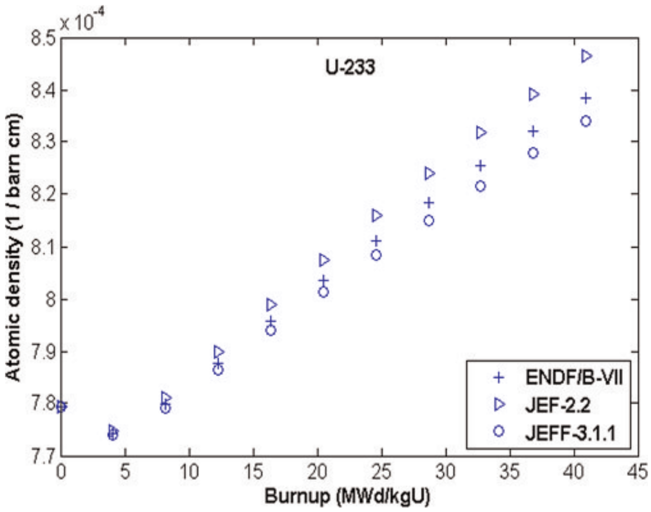


Fig. 4. Effective multiplication factor



(a)



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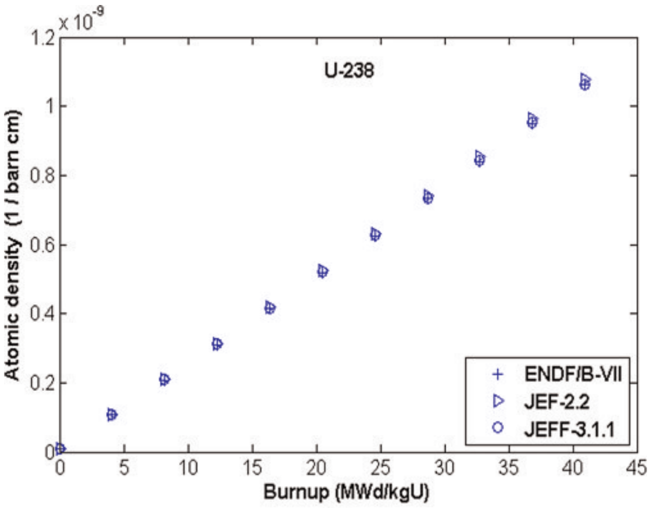
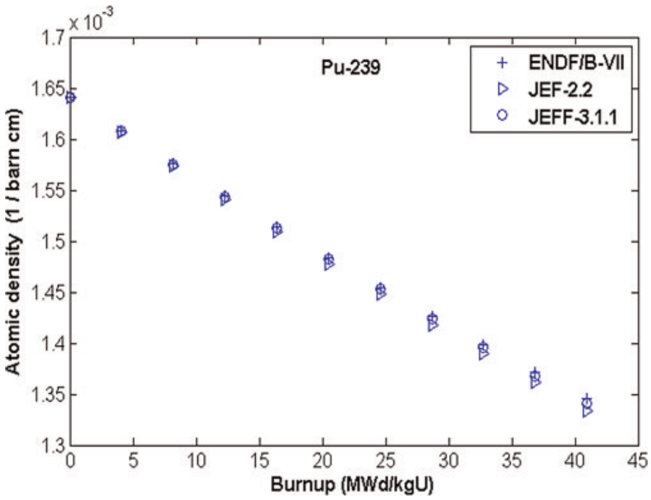


(c)



(d)

Fig. 5. The atomic density change for (a) ^{232}Th (b) ^{233}U (c) ^{238}U (d) ^{239}Pu

tion library for the calculations ENDF/B-VII, JEF-2.2 and JEFF-3.1.1 have been selected. The neutronic characteristic is important when ADTR is operated as subcritical. The neutronic performance of the target, fuel 1 and fuel 2 are shown in Fig. 2 and Fig. 3 respectively. These calculations were carried out to examine the neutronic properties of ADTR and methods for the evaluation of reactor parameters including the reaction rate distribution. The neutronic calculations were achieved for neutron energy according to neutron flux per lethargy in the Pb–Bi target, fuel 1 and fuel 2.

The simulations were performed in order to obtain burn-up characteristics of ADTR. The Serpent burnup calculation was completed using the CRAM method in less than 16 h on a double-processor 2.4 GHz Intel Xeon PC workstation. An irradiation period of 600 days was used at 2000 MWth ADTR. The irradiation history has been obtained for 20.000 source particles. According to burnup, Fig. 4 shows effective multiplication factors for different libraries. There is a significant difference in different libraries for the operation period. The k_{eff} is between 0.93 and 0.97. The atomic density change of ^{232}Th, ^{233}U, ^{238}U and ^{239}Pu is presented in Fig. 5.

7 Conclusions

In this study, our knowledge has been increased with regard to thorium fuels in Accelerator Driven Thorium Systems (ADTR) by means of the Serpent Monte Carlo Code. The Serpent Monte Carlo code has been used successfully in realistic full scale assembly burnup calculations to obtain the best knowledge on neutron interactions. An ADTR has been designed using Serpent 1.1.16 for burning ^{232}Th and ^{233}U fuels including mixed minor actinide. The mass conversion was performed for ^{232}Th, ^{233}U, ^{238}U and ^{239}Pu during irradiation. The Th-based mixed fuels including nuclear waste are expected to have superior transmutation properties. ADTR should be safer than conventional fast breeder reactors. Our calculations show that the effective multiplication factor can increase from 0.93 to 0.97 for different libraries during the reactor operation period. Thus, they are less likely to become supercritical. Consequently, since uranium reserves are limited on Earth, these reactors can be a great source of energy for the future and also decrease nuclear waste.

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